XPS and NEXAFS Spectroscopy Study of Pentacene Adsorption on Epitaxial Graphene and BN

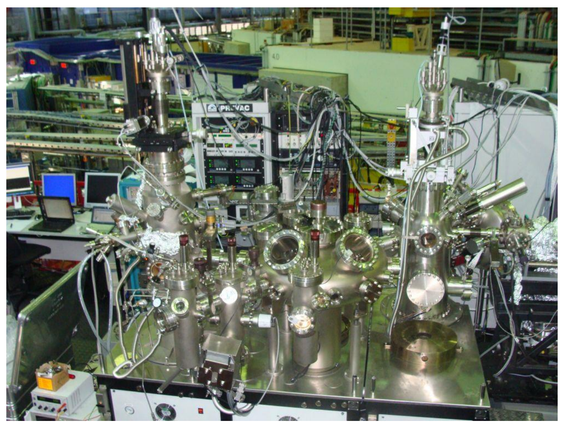
A. Nefedov[1], W. Zhang[1,2], A. Fedorov[3], N. Verbitskiy[4], A. Grüneis[3], and Ch. Wöll[1]

[1]Institute of Functional Interfaces, Karlsruhe Institute of Technology, Germany
[2]National Synchrotron Radiation Laboratory, Hefei, People Republic of China
[3]II. Physikalisches Institut, Universität zu Köln, Köln, Germany
[4]Vienna University, Vienna, Austria

Motivation

- Pentacene and graphene are promice candidates for organic electronics:
  - behaviour on the interface between them is very important
  - flat orientation of the first pentacene layer is necessary
- Fundamental understanding of the interaction on graphene/metal interface:
  - „weak“ or „strong“
  Pentacene as a probe molecule
  Comparison of EG/Ni(111) *vs.* EG/Au/Ni(111) and h-BN/Au/Ni(111)
- Possible interaction of pentacene with metal substrate through graphene - ?
  Presence of „surface phase“ similar to chemisorbed pentacene on Ag(111)
  [*Käfer et al, CPL*, **442** (2007) 376–383]
- Additional challenge:
  Evaluation of C *K*-edge NEXAFS spectra for organic/graphene systems

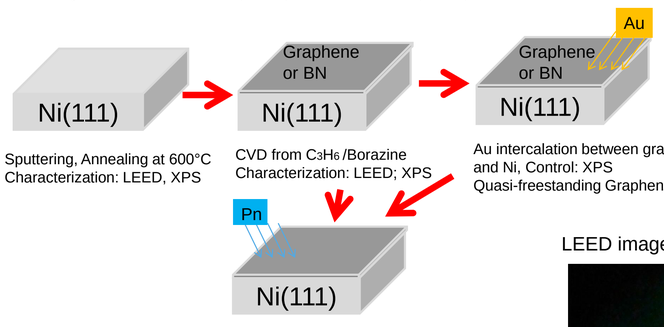
XPS/NEXAFS endstation @ HESGM (BESSY II)



Partial electron yields (PEY) mode for NEXAFS with home-made MCP detector.
SRXPS with VG Scienta R3000 analyzer.

Sample preparation and layout of the experiment

Used systems: EG/Ni(111), EG/Au/Ni(111) and h-BN/Au/Ni(111)



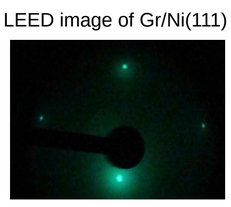
Sputtering, Annealing at 600°C
Characterization: LEED, XPS

CVD from C_3H_6 /Borazine
Characterization: LEED; XPS

Au intercalation between graphene and Ni, Control: XPS
Quasi-freestanding Graphene/BN

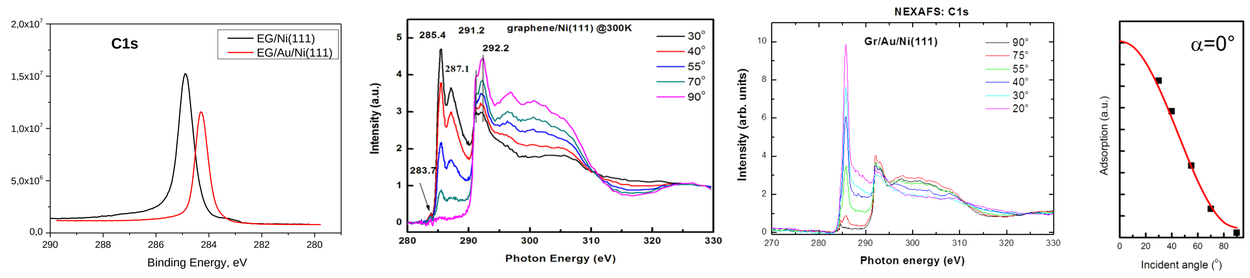
Pn deposition
Characterization: XPS, NEXAFS

LEED image of Gr/Ni(111)



Pn thickness calibration with QCM

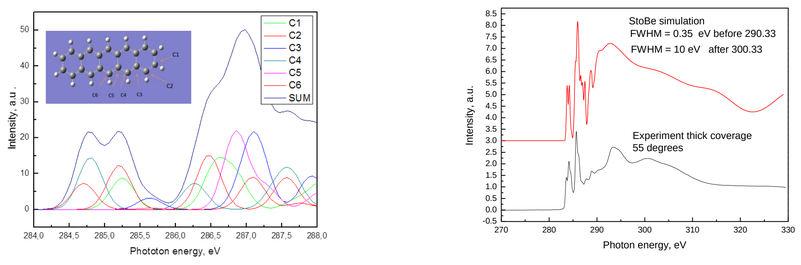
XPS and NEXAFS: Comparison of Gr/Ni and Gr/Au/Ni



XPS (left panel) and NEXAFS characterizations of single layer of graphene prepared by C_2H_4 cracking on Ni(111) surface before and after au intercalation (central panels). The state at 287.1eV denotes strong hybridization between graphene with Ni(111).

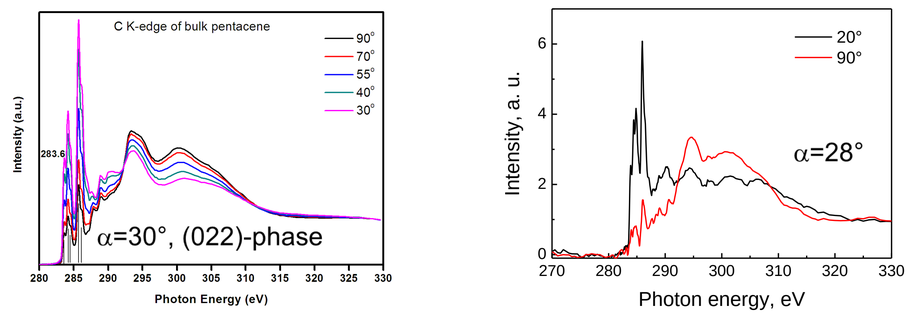
Angle dependence of NEXAFS Intensity (right panel) shows a highly parallel graphene layer on Ni(111).

Simulation of NEXAFS spectra of Pn molecule (in gas phase)

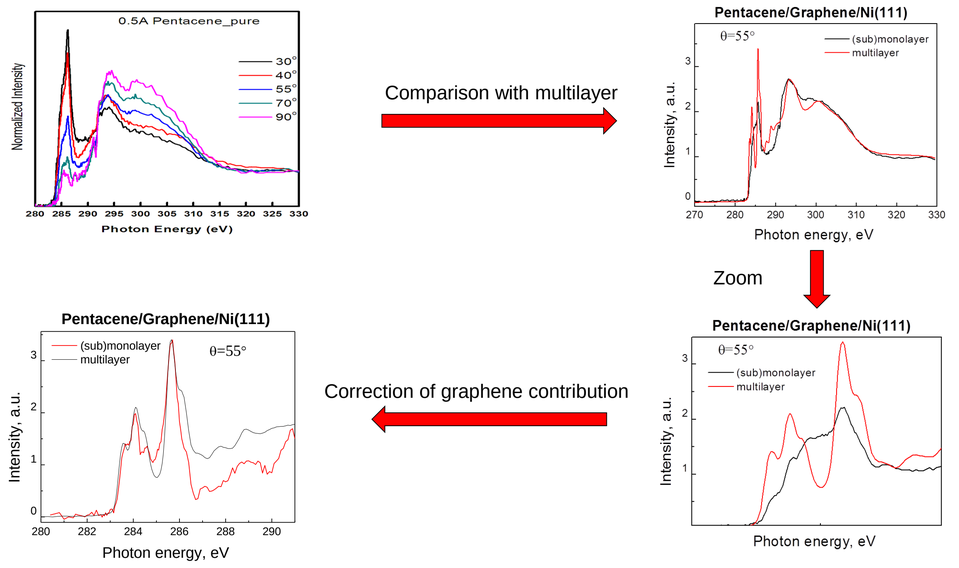


Atomic specific XAS calculations for carbon K-edge of Pn molecule using StoBe package.

Pentacene multilayer on graphene and h-BN

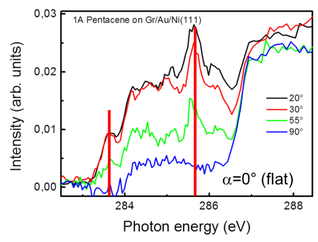


Pn submonolayer on EG/Ni(111): correction of graphene contribution

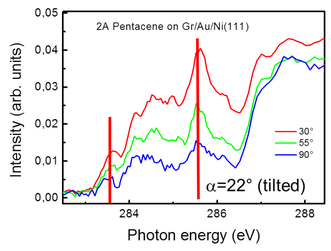


No hybridization – „weak“ interaction! Flat orientation of the first Pn layer!

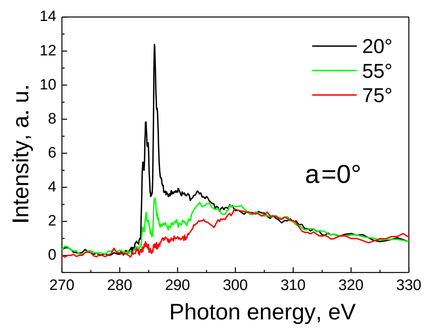
EG/Au/Ni(111) Submonolayer



Growth of the second layer



Pentacene on h-BN: (sub)monolayer



Conclusions

- Flat orientation of pentacene at submonolayer coverages – independent on substrate configuration
- Direct growth of tilted phase already for the second layer
- Weak interaction between pentacene and graphene
- No „surface phase“ was observed – no interaction with metal substrate through EG layer